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MODELING OF THIN-FILM GaAs GROWTH

By

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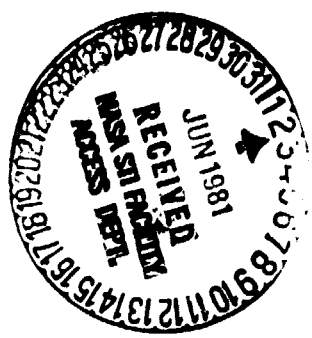

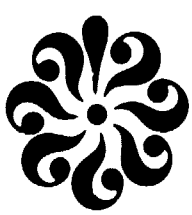

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INTRODUCTION

During this phase of the project (February 1-May 15, 1981), a literature survey was conducted of articles relating to the Monte Carlo simulation of crystal growth. A list of references being reviewed is presented in the next section.

Two approaches to the analysis of crystal growth currently exist: (1) a statistical analysis of the surface mechanics and (2) a thermodynamical-chemical analysis of vapor deposits. It is the goal of this research to produce a Monte Carlo computer program which will be useful in the analysis of crystal growth. Hence, we are primarily interested in the statistical analysis approach in our modeling of crystal growth phenomena. In an attempt to create a useful model of crystal growth processes we will borrow extensively from the thermodynamical-chemical analysis and try to incorporate many thermodynamical concepts into the computer model.

The research is progressing along the lines of determining what statistical measures will be of laboratory use in the analysis of crystal growth. At present the following measures are being considered: (1) a roughness factor; (2) growth rates in one region compared with growth rates in another region, which can be used to compare the effect of initial substrate geometry on crystal growth; (3) a geometrical "picture" of the crystal growth at any time, indicating clustering; (4) size and number of "average clusters;" (5) BET adsorption isotherm measures θ, p/p^* where θ = total number of particles adsorbed/total sites available and p/p^* is a vapor pressure ratio; and (6) other abstract measures which may prove to be useful.

In addition to determining statistical measures, it is necessary to decide what geometrical and physical parameters and variables should be

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included in any Monte Carlo simulation. Some of these variables will be assumed random, and other variables will be calculated and averaged during many simulations of crystal growth. Other quantities will be considered as parameters and assigned fixed values during the Monte Carlo process. Once the variables and parameters are chosen, it is necessary to assign probability distributions to the random variables, as these distributions will ultimately dictate the behavior of the Monte Carlo model. These factors are currently under study.

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